Generalized Einstein relation in conductors with a large built-in field

Sergey A. Ktitorov
Ioffe Institute, Polytechnicheskaya str. 26, 194021 St. Petersburg,
Russia and State Electrotechnical University, Prof. Popov str. 5, 197376 St. Ptersburg, Russia

Generalized Einstein relation between the mobility and diffusion in conductors with a large built-in field near the thermodynamic equilibrium has been derived.

The mobility and diffusion coefficients depend on the particle energy. When the system under consideration is in the inequilibrium state and the current does not vanish, the electons are hot and their energy is determined by the balance of power, which electrons acquire from the electric field and transfere to the thermostat. Mobility is determined by the mean kinetic energy of electrons and within the framework of the quasi-hydrodynamic approximation can be considered as a function of the local electric field, if inhomogeneities are spread along the current lines [1] (this is the case for N-shape current-voltage characteristics). Attempts to generalize the Einstein relation are directed mainly to analysis of strongly inequilibrium state (see [2], for instance). In the opposite case of S-shape charaterisitics the mobility can be considered as a function of the local current. We encounter quite different situation, when the system is near the thermodynamic equilibrium, but the built-in electric field is strong enough so that the mobility depends mainly on the potential energy: $\mu = \mu(\phi)$. Therefore, the diffusion coefficient depends on the potential as well: $D = D(\phi)$. We consider here a one-dimensional distribution of the electric field and the electronic density. The total current reads:

$$j = -en(x)\,\mu[\phi(x)]\frac{d\phi}{dx} - e\frac{d}{dx}[D(\phi)\,n(x)], \quad , E = -d\phi/dx, \quad \frac{dj}{dx} = 0. \tag{1}$$

We have in the thermodynamic equilibrium:

$$j = 0, \quad n(x) = n_0 e^{-\frac{e\phi}{T}}. \tag{2}$$

Carrying out differetiation in (1) we have

$$j = -en(x)\,\mu[\phi(x)]\frac{d\phi}{dx} - e\frac{dD}{d\phi}n(x)\frac{d\phi}{dx} - eD(\phi)\frac{dn}{d\phi}\frac{d\phi}{dx}, \tag{3}$$

where $\frac{dn}{d\phi} = -\frac{e}{T}n$. Thus, we obtain the differential equation for the diffusion coefficient:

$$\frac{dD}{d\phi} + \frac{d\log n}{d\phi}D + \mu(\phi) = 0 \tag{4}$$

or

$$\frac{dD}{d\phi} - \frac{e}{T}D + \mu(\phi) = 0$$

Let us denote $\mu(\phi = 0) \equiv \mu_0$. Then we can introduce the dimensionless variables:

$$\widetilde{\mu} = \frac{\mu}{\mu_0}, \quad \psi = \frac{e\phi}{T}, \quad \widetilde{D} = \frac{eD}{\mu_0 T}. \tag{5}$$

We obtain the following differential equation for the dimensionless diffusion coefficient:

$$\frac{d\widetilde{D}}{d\psi} - \widetilde{D} + \widetilde{\mu}(\psi) = 0 \tag{6}$$

Formulae (5) show that the dimensional factor in the diffusion coefficient has the standart form $D/\widetilde{D} = \mu_0 T/e$. However, the relation between the diffusion coefficient and the mobility is non-local, as it can be seen from the equation (6). The solution of this equation with the initial condition $\widetilde{D}(0) = \widetilde{D}_0$ reads:

$$\widetilde{D}(\psi) = \exp(\psi)\left[\widetilde{D}_0 - \int_0^{\psi} dz\,\widetilde{\mu}(z)\exp(-z)\right] \tag{7}$$

Let us consider the trivial case of constant mobility: $\mu = \mu_0$, and, therefore, $\widetilde{\mu} = 1$, $\widetilde{D}_0 = 1$. The solution (7) takes the form:

$$\widetilde{D}\left(\psi\right) = \exp\left(\psi\right)\left[1 - \int_0^{\psi} dz \exp\left(-z\right)\right] = 1. \tag{8}$$

This calculation confirms consistency of our description.

Now we consider the case of the exponential law mobility dependence $\widetilde{\mu} = \exp\left(a\psi\right)$.

$$\widetilde{D}\left(\psi\right) = \exp\left(\psi\right) - \exp\left(\psi\right)\int_0^{\psi} dz \exp((a-1)z) = \frac{a\exp\left(\psi\right)}{a-1} - \frac{\exp\left(a\psi\right)}{a-1} \tag{9}$$

This expression tends to unity, when $a \longrightarrow 0$ or $\psi \longrightarrow 0$. The diffusion coefficient vanishes identically at $a - 1$.

Let us consider now the case of linear dependence of the mobility on the potential: $\widetilde{\mu} = 1 + a\psi$. Then we have:

$$\widetilde{D}\left(\psi\right) = \exp\left(\psi\right)\left[1 - \int_0^{\psi} dz \exp\left(-z\right)\right] = 2 + \psi - \exp\left(\psi\right). \tag{10}$$

Thus, we see that the diffusion vs mobility relation near the equilibrium is generically non-local. The conventional Einstein relation $D = \mu T/e$ is valid in the limit of low built-in potential.

[1] A.F. Volkov, Sh.M. Kogan. Uspehi Fizicheskih Nauk, V. **96**, 633 (1968).
[2] V.Blickle, T. Speck, C. Lutz, U. Seifert, C. Bechinger. Phys. Rev. Lett. **98**, 210601 (2007).